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Methyl {2-[(3-phenyl-1,2,4-oxadiazol-5-yl)methoxy]phenyl}acetate

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The title compound, $C_{18}H_{16}N_2O_4$, was synthesized by the reaction of methyl (2-hydroxyphenyl)acetate and 5-chloromethyl-3-phenyl-1,2,4-oxadiazole. In the crystal structure, there are weak intermolecular C—H$\cdots$O hydrogen bonds and weak C—H$\cdots\pi$(arene) interactions.

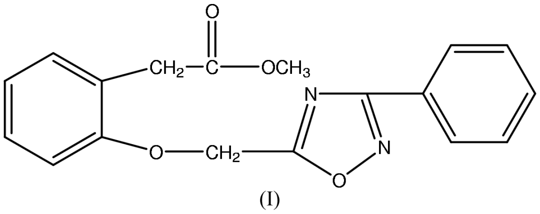
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.056
wR factor = 0.186
Data-to-parameter ratio = 14.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

1,2,4-Oxadiazole derivatives are of great interest because of their biological properties. Some derivatives of 1,2,4-oxadiazoles have intrinsic analgesic (Terashita *et al.*, 2002), anti-inflammatory (Nicolaides *et al.*, 1998), and antipicornaviral (Romero, 2001) properties and are efficient as agonists [*e.g.* formuscarinic (Macor *et al.*, 1996), adrenergic agents (Quagliato & Andrae, 2002) and 5-hydroxytryptamine (Gur *et al.*, 2001)] and antagonists [*e.g.* for angiotension (Naka & Kubo, 1999 and adhesion (Juraszyk *et al.*, 1997)] for different receptors.



(I)

The molecular structure of (I) is shown in Fig. 1 and the bond lengths and angles are given in Table 1. In the crystal structure, molecules are linked by C—H$\cdots$O hydrogen bonds and there is also an intermolecular contact which indicates a weak C—H$\cdots\pi$(arene) interaction. Full details of the hydrogen bonding are given in Table 2 (see also Fig. 2 and Fig. 3). The combination of both types of weak interactions generates a three-dimensional network.

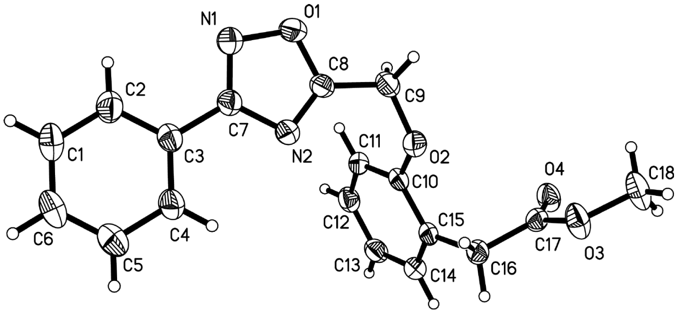


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level

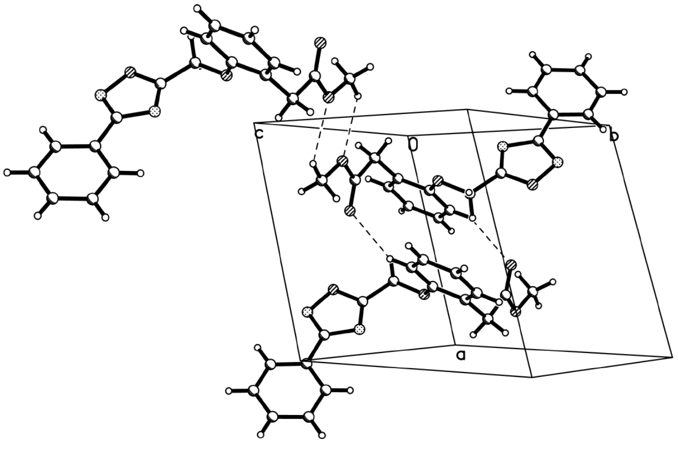


Figure 2
The crystal structure of (I). Dashed lines indicate weak C—H···O hydrogen bonds.

Experimental

Methyl (2-hydroxyphenyl)acetate (20 mmol) was dissolved in acetone (20 ml) and potassium carbonate (30 mmol) was added in one portion. 5-Chloro-3-phenyl-1,2,4-oxadiazole (20 mmol) in acetone (20 ml) was added to this mixture. The resulting mixture was refluxed for 4 h, then concentrated under reduced pressure to afford crude compound (I). Pure compound (I) was obtained by recrystallization from ethyl acetate (m.p. 354–355 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution. Spectroscopic analysis, ^{1}H NMR (CDCl$_3$, p.p.m.): 8.12–8.13 (*m*, 2H), 7.50–7.55 (*m*, 3H), 7.26–7.32 (*m*, 2H), 7.01–7.06 (*m*, 2H), 5.39 (*s*, 2H), 3.77 (*s*, 2H), 3.73 (*s*, 3H)).

Crystal data

$C_{18}H_{16}N_2O_4$
$M_r = 324.33$
Triclinic, $P\overline{1}$
$a = 8.7850$ (18) Å
$b = 9.848$ (2) Å
$c = 10.345$ (2) Å
$\alpha = 77.90$ (3)°
$\beta = 79.12$ (3)°
$\gamma = 67.39$ (3)°
$V = 802.0$ (3) Å^3
$Z = 2$
$D_x = 1.343$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 10$–13°
$\mu = 0.10$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.40 × 0.30 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (*SHELXTL*; Siemens, 1996)
$T_{\min} = 0.963$, $T_{\max} = 0.972$
3347 measured reflections
3129 independent reflections
2141 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.022$
$\theta_{\max} = 26.0°$
$h = 0 \rightarrow 10$
$k = -11 \rightarrow 12$
$l = -12 \rightarrow 12$
3 standard reflections every 200 reflections intensity decay: negligible

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.186$
$S = 1.17$
3129 reflections
217 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.076P)^2 + 0.34P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.23$ e Å^{-3}
$\Delta\rho_{\min} = -0.32$ e Å^{-3}

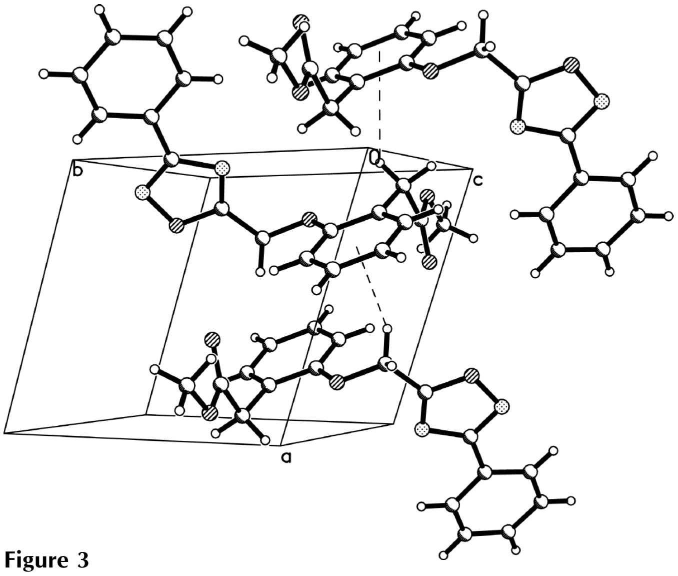


Figure 3
The C—H···π(arene) interactions in (I), shown as dashed lines.

Table 1
Selected geometric parameters (Å, °).

O1—C8	1.326 (3)	N1—C7	1.296 (4)
O1—N1	1.418 (3)	N2—C8	1.291 (3)
O2—C10	1.375 (3)	N2—C7	1.383 (4)
O2—C9	1.418 (3)	C8—C9	1.497 (4)
O3—C17	1.328 (3)	C15—C16	1.504 (4)
O3—C18	1.450 (4)	C16—C17	1.499 (4)
O4—C17	1.200 (3)		
C8—O1—N1	106.2 (2)	N2—C8—O1	113.8 (2)
C10—O2—C9	118.2 (2)	N2—C8—C9	131.1 (3)
C17—O3—C18	116.0 (2)	O2—C9—C8	112.3 (2)
C7—N1—O1	103.3 (2)	C17—C16—C15	112.7 (2)
C8—N2—C7	102.5 (2)	O4—C17—O3	122.9 (2)
N1—C7—N2	114.3 (3)	O4—C17—C16	125.7 (3)
N1—C7—C3	122.3 (3)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11A···O4$^{\rm i}$	0.93	2.47	3.319 (4)	152
C18—H18A···O3$^{\rm ii}$	0.96	2.55	3.272 (5)	132
C9—H9A···Cg3$^{\rm i}$	0.97	2.81	3.503 (4)	129

Symmetry codes: (i) $1 - x, -y, -z$; (ii) $-x, -y, 1 - z$. Cg3 is the centroid of the ring C10–C15.

All H atoms were placed in calculated positions, with C—H distances in the range 0.93–0.97 Å. They were included in the riding-model approximation, with $U_{\rm iso} = 1.2U_{\rm eq}$(C) or $1.5_{\rm eq}$(C$_{\rm Me}$).

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *XCAD*4 (Harms, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL*97.

References

Enraf–Nonius (1989). *CAD*-4 *Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.

Gur, E., Dremencov, E., Lerer, B. & Newman, M. E. (2001). *Eur. J. Pharmacol.* **411**, 115–122.

Harms, K. (1995). *XCAD*4. University of Marburg, Germany.

Juraszyk, H., Gante, J., Wurziger, H., Bernotat-Danielowski, S. & Melzer, G. (1997). PCT Int. Appl. No. 9744333.

Macor, J. E., Ordway, T., Smith, R. L., Verhoest, P. R. & Mack, R. A. (1996). *J. Org. Chem.* **61**, 3228–3229.

Naka, T. & Kubo, K. (1999). *Curr. Pharm. Des*. **5**, 453–472.

Nicolaides, D. N., Fylaktakidou, K. C., Litinas, K. E. & Hadjipavlou-Litina, D. (1998). *Eur. J. Med. Chem.* **33**, 715–724.

Quagliato, D. A. & Andrae, P. M. (2002). PCT Int. Appl. WO 0206250.

Romero, J. R. (2001). *Expert Opin. Invest. Drugs*, **10**, 369–379.

Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

Siemens (1996). *SHELXTL*. Version 5.06. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Terashita, Z., Naruo, K. & Morimoto, S. (2002). PCT Int. Appl. WO 0260439.